



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:59 AM UTC

PDB ID : 1RAL / pdb_00001ral
Title : THREE-DIMENSIONAL STRUCTURE OF RAT LIVER 3ALPHA-HYDROXYSTEROID(SLASH)DIHYDRODIOL DEHYDROGENASE: A MEMBER OF THE ALDO-KETO REDUCTASE SUPERFAMILY
Authors : Hoog, S.S.; Pawlowski, J.E.; Alzari, P.M.; Penning, T.M.; Lewis, M.
Deposited on : 1994-02-04
Resolution : 3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

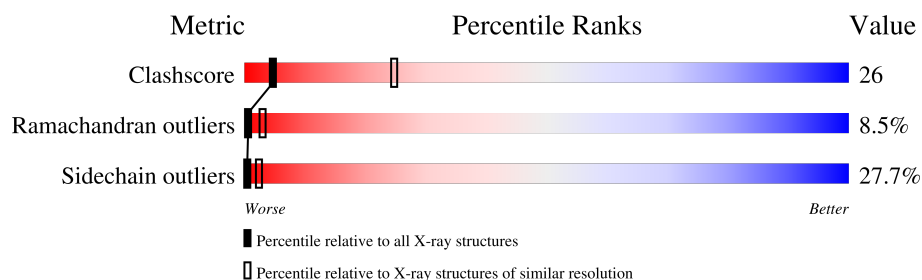
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

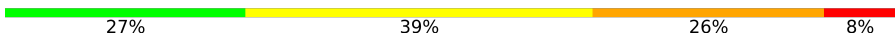
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	308	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3029 atoms, of which 558 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 3-ALPHA-HYDROXYSTEROID DEHYDROGENASE.

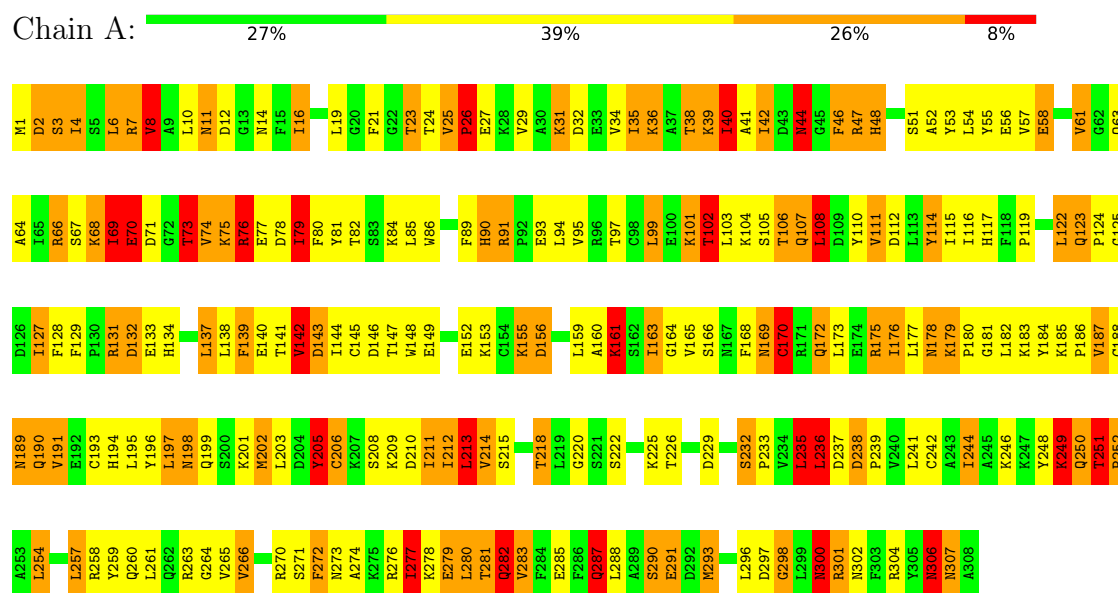
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	308	3029	1580	558	417	460	14	127	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

• Molecule 1: 3-ALPHA-HYDROXYSTEROID DEHYDROGENASE



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	51.30Å 89.50Å 143.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-3.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.220 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3029	wwPDB-VP
Average B, all atoms (Å ²)	13.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.22	14/2520 (0.6%)	2.31	142/3404 (4.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	212	ILE	CA-CB	9.63	1.64	1.53
1	A	251	THR	CA-CB	7.58	1.65	1.53
1	A	127	ILE	CA-CB	7.36	1.63	1.54
1	A	142	VAL	CA-CB	6.77	1.63	1.54
1	A	236	LEU	CA-CB	6.38	1.61	1.52
1	A	29	VAL	CA-CB	5.82	1.60	1.54
1	A	35	ILE	CA-CB	5.80	1.62	1.54
1	A	254	LEU	CA-CB	-5.79	1.44	1.53
1	A	187	VAL	CA-CB	5.74	1.62	1.54
1	A	8	VAL	CA-CB	5.74	1.63	1.55
1	A	79	ILE	CA-CB	5.70	1.61	1.54
1	A	25	VAL	CA-CB	5.50	1.61	1.54
1	A	82	THR	CA-CB	5.35	1.61	1.53
1	A	102	THR	CA-CB	5.03	1.61	1.53

All (142) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	273	ASN	CA-CB-CG	15.37	127.97	112.60
1	A	6	LEU	CA-C-O	-10.49	109.67	120.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	238	ASP	CA-CB-CG	10.10	122.70	112.60
1	A	132	ASP	CA-CB-CG	9.36	121.96	112.60
1	A	249	LYS	N-CA-C	8.98	123.42	109.96
1	A	2	ASP	CA-CB-CG	-8.97	103.63	112.60
1	A	273	ASN	CB-CG-ND2	8.68	129.41	116.40
1	A	32	ASP	N-CA-C	8.40	122.35	110.68
1	A	63	GLN	CA-C-O	-8.20	112.39	121.00
1	A	149	GLU	N-CA-C	-7.92	101.36	111.02
1	A	177	LEU	N-CA-CB	-7.88	97.17	110.41
1	A	189	ASN	CA-CB-CG	-7.86	104.74	112.60
1	A	104	LYS	CA-CB-CG	7.80	129.70	114.10
1	A	46	PHE	CA-CB-CG	7.55	121.35	113.80
1	A	211	ILE	N-CA-CB	-7.51	102.54	110.95
1	A	273	ASN	OD1-CG-ND2	-7.45	115.15	122.60
1	A	254	LEU	CA-C-O	-7.40	113.05	120.82
1	A	125	GLY	O-C-N	7.39	131.02	123.92
1	A	235	LEU	O-C-N	-7.36	114.32	122.12
1	A	78	ASP	CA-CB-CG	7.30	119.90	112.60
1	A	279	GLU	CA-CB-CG	7.24	128.59	114.10
1	A	306	ASN	CB-CG-ND2	7.17	127.15	116.40
1	A	2	ASP	N-CA-C	7.16	121.52	110.20
1	A	149	GLU	CA-CB-CG	7.16	128.43	114.10
1	A	2	ASP	O-C-N	7.16	131.46	123.01
1	A	23	THR	CA-C-O	-7.04	111.61	120.28
1	A	218	THR	N-CA-CB	-6.93	99.93	110.12
1	A	291	GLU	N-CA-C	-6.93	103.65	111.14
1	A	208	SER	CA-CB-OG	6.86	124.81	111.10
1	A	281	THR	N-CA-C	-6.85	104.39	112.89
1	A	141	THR	N-CA-C	6.81	119.94	108.23
1	A	44	ASN	CA-CB-CG	-6.78	105.82	112.60
1	A	108	LEU	N-CA-C	-6.70	100.61	110.52
1	A	139	PHE	CA-C-O	-6.68	113.63	120.71
1	A	197	LEU	N-CA-C	-6.66	96.61	110.80
1	A	301	ARG	CA-C-N	6.65	134.25	121.54
1	A	301	ARG	C-N-CA	6.65	134.25	121.54
1	A	129	PHE	CA-CB-CG	6.65	120.45	113.80
1	A	181	GLY	N-CA-C	6.65	123.19	113.48
1	A	215	SER	N-CA-C	6.61	119.94	108.76
1	A	249	LYS	CA-C-N	6.56	134.07	121.54
1	A	249	LYS	C-N-CA	6.56	134.07	121.54
1	A	270	ARG	N-CA-C	-6.55	100.51	109.95
1	A	183	LYS	CA-CB-CG	6.52	127.14	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	139	PHE	CA-CB-CG	6.49	120.29	113.80
1	A	290	SER	N-CA-C	6.46	119.14	111.71
1	A	195	LEU	N-CA-C	6.45	124.53	110.80
1	A	7	ARG	N-CA-C	6.40	119.97	109.85
1	A	1	MET	CA-C-N	-6.37	112.31	121.42
1	A	1	MET	C-N-CA	-6.37	112.31	121.42
1	A	8	VAL	N-CA-C	6.35	117.51	108.42
1	A	306	ASN	OD1-CG-ND2	-6.35	116.25	122.60
1	A	249	LYS	O-C-N	6.33	130.72	122.93
1	A	287	GLN	CB-CG-CD	6.29	123.30	112.60
1	A	127	ILE	N-CA-CB	6.28	119.38	111.46
1	A	133	GLU	CA-CB-CG	6.23	126.55	114.10
1	A	76	ARG	N-CA-C	6.20	124.01	110.80
1	A	74	VAL	O-C-N	6.15	129.75	122.36
1	A	186	PRO	N-CA-C	6.12	120.81	111.15
1	A	138	LEU	N-CA-C	-6.07	100.66	109.59
1	A	123	GLN	CA-C-N	6.07	126.39	119.83
1	A	123	GLN	C-N-CA	6.07	126.39	119.83
1	A	213	LEU	CA-C-O	6.06	127.99	121.02
1	A	74	VAL	CB-CA-C	-6.03	102.94	111.38
1	A	178	ASN	CA-CB-CG	6.03	118.63	112.60
1	A	202	MET	N-CA-C	-6.02	105.02	112.90
1	A	248	TYR	N-CA-C	-5.99	97.36	108.02
1	A	300	ASN	N-CA-C	5.99	123.55	110.80
1	A	169	ASN	CA-CB-CG	5.96	118.56	112.60
1	A	64	ALA	CA-C-O	-5.95	114.24	120.55
1	A	208	SER	N-CA-C	-5.93	104.81	111.28
1	A	236	LEU	CA-CB-CG	5.93	137.05	116.30
1	A	53	TYR	O-C-N	5.89	128.13	122.07
1	A	176	ILE	O-C-N	5.87	129.91	122.57
1	A	80	PHE	CA-C-O	-5.85	114.05	120.30
1	A	235	LEU	N-CA-C	5.83	117.64	111.28
1	A	261	LEU	O-C-N	5.80	128.13	122.09
1	A	198	ASN	CA-CB-CG	5.80	118.40	112.60
1	A	48	HIS	CA-CB-CG	5.79	119.59	113.80
1	A	47	ARG	CB-CG-CD	5.76	124.54	111.30
1	A	307	ASN	CB-CG-ND2	5.76	125.03	116.40
1	A	252	PRO	N-CA-C	5.73	124.28	112.47
1	A	190	GLN	CA-CB-CG	5.71	125.53	114.10
1	A	164	GLY	CA-C-O	-5.70	116.02	121.38
1	A	307	ASN	OD1-CG-ND2	-5.65	116.95	122.60
1	A	21	PHE	CA-CB-CG	5.63	119.43	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	156	ASP	N-CA-CB	-5.62	101.26	110.14
1	A	198	ASN	OD1-CG-ND2	-5.62	116.98	122.60
1	A	163	ILE	CA-C-O	-5.62	115.12	121.75
1	A	104	LYS	CB-CA-C	-5.56	102.15	110.88
1	A	251	THR	CA-C-N	5.56	126.78	119.84
1	A	251	THR	C-N-CA	5.56	126.78	119.84
1	A	3	SER	CA-C-N	5.54	131.93	121.97
1	A	3	SER	C-N-CA	5.54	131.93	121.97
1	A	69	ILE	CA-C-O	5.52	127.68	120.78
1	A	285	GLU	CA-CB-CG	5.51	125.13	114.10
1	A	143	ASP	CA-CB-CG	5.49	118.09	112.60
1	A	91	ARG	CA-C-N	5.46	125.11	119.05
1	A	91	ARG	C-N-CA	5.46	125.11	119.05
1	A	117	HIS	CA-C-O	-5.45	113.36	119.79
1	A	11	ASN	O-C-N	5.45	129.83	122.59
1	A	172	GLN	OE1-CD-NE2	-5.44	117.16	122.60
1	A	105	SER	CA-C-O	-5.41	114.81	120.55
1	A	16	ILE	CA-C-N	5.39	125.33	119.78
1	A	16	ILE	C-N-CA	5.39	125.33	119.78
1	A	147	THR	N-CA-C	-5.38	105.50	111.36
1	A	264	GLY	O-C-N	5.36	129.66	122.70
1	A	31	LYS	CA-CB-CG	5.36	124.81	114.10
1	A	185	LYS	CA-C-N	5.34	125.34	119.90
1	A	185	LYS	C-N-CA	5.34	125.34	119.90
1	A	282	GLN	CA-C-O	-5.34	113.03	119.49
1	A	266	VAL	CA-C-N	5.31	125.51	120.31
1	A	266	VAL	C-N-CA	5.31	125.51	120.31
1	A	175	ARG	CA-CB-CG	5.31	124.71	114.10
1	A	39	LYS	CA-C-O	-5.30	115.24	120.70
1	A	133	GLU	N-CA-CB	5.29	119.42	110.49
1	A	206	CYS	O-C-N	5.28	127.51	122.07
1	A	73	THR	N-CA-C	-5.26	105.68	112.68
1	A	307	ASN	O-C-N	5.26	129.37	123.27
1	A	70	GLU	N-CA-C	-5.24	99.64	110.80
1	A	155	LYS	O-C-N	5.24	127.75	122.09
1	A	26	PRO	N-CA-CB	-5.23	97.75	103.25
1	A	260	GLN	OE1-CD-NE2	-5.17	117.42	122.60
1	A	114	TYR	N-CA-C	-5.17	100.60	109.24
1	A	277	ILE	N-CA-C	-5.16	105.47	113.16
1	A	70	GLU	CA-CB-CG	5.16	124.42	114.10
1	A	278	LYS	CB-CA-C	-5.16	101.27	110.70
1	A	36	LYS	CB-CG-CD	5.15	123.15	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	205	TYR	CA-C-N	5.14	127.13	120.44
1	A	205	TYR	C-N-CA	5.14	127.13	120.44
1	A	172	GLN	N-CA-C	-5.13	106.28	112.54
1	A	170	CYS	N-CA-CB	-5.10	101.87	110.49
1	A	3	SER	CA-C-O	-5.09	115.38	120.77
1	A	21	PHE	N-CA-CB	-5.07	102.41	111.08
1	A	272	PHE	N-CA-C	-5.05	100.05	110.80
1	A	142	VAL	CB-CA-C	5.05	119.57	111.29
1	A	285	GLU	N-CA-CB	-5.04	102.69	110.46
1	A	214	VAL	N-CA-C	-5.04	101.21	108.87
1	A	244	ILE	CB-CA-C	-5.04	105.44	112.04
1	A	301	ARG	N-CA-C	-5.04	104.86	111.96
1	A	161	LYS	N-CA-C	5.03	121.51	110.80
1	A	297	ASP	N-CA-C	-5.03	106.36	113.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	232	SER	Peptide
1	A	251	THR	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2471	558	2489	123	0
All	All	2471	558	2489	123	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 26.

All (123) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:VAL:HG12	1:A:213:LEU:HD21	1.56	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:LEU:HG	1:A:283:VAL:HG11	1.58	0.86
1:A:119:PRO:HG2	1:A:172:GLN:HE21	1.41	0.83
1:A:193:CYS:SG	1:A:198:ASN:HA	2.26	0.75
1:A:236:LEU:HD21	1:A:276:ARG:HH21	1.52	0.75
1:A:220:GLY:HA3	1:A:235:LEU:HD21	1.71	0.72
1:A:68:LYS:HB3	1:A:74:VAL:HG23	1.74	0.68
1:A:91:ARG:NH2	1:A:140:GLU:HB3	2.08	0.68
1:A:196:TYR:HA	1:A:300:ASN:HA	1.74	0.67
1:A:249:LYS:HE2	1:A:250:GLN:HG2	1.75	0.67
1:A:44:ASN:ND2	1:A:281:THR:HG21	2.10	0.67
1:A:24:THR:HG22	1:A:25:VAL:H	1.60	0.66
1:A:254:LEU:HD23	1:A:283:VAL:HG12	1.77	0.66
1:A:304:ARG:HG2	1:A:306:ASN:O	1.96	0.66
1:A:103:LEU:HD21	1:A:111:VAL:HG22	1.78	0.64
1:A:67:SER:O	1:A:70:GLU:HB3	1.98	0.63
1:A:10:LEU:HB3	1:A:14:ASN:O	1.99	0.63
1:A:131:ARG:HA	1:A:137:LEU:HA	1.81	0.63
1:A:97:THR:O	1:A:101:LYS:HB2	2.00	0.62
1:A:8:VAL:HG13	1:A:16:ILE:CG2	2.30	0.61
1:A:123:GLN:OE1	1:A:124:PRO:HD2	2.00	0.61
1:A:214:VAL:HG22	1:A:266:VAL:HB	1.82	0.61
1:A:38:THR:HG21	1:A:61:VAL:HG22	1.84	0.60
1:A:71:ASP:HB2	1:A:73:THR:OG1	2.01	0.60
1:A:84:LYS:HE3	1:A:115:ILE:HD11	1.85	0.59
1:A:102:THR:HG22	1:A:103:LEU:HD23	1.84	0.58
1:A:8:VAL:HG13	1:A:16:ILE:HG23	1.85	0.58
1:A:34:VAL:HG11	1:A:57:VAL:HG11	1.85	0.58
1:A:41:ALA:O	1:A:46:PHE:HB2	2.04	0.57
1:A:115:ILE:HD12	1:A:166:SER:OG	2.05	0.57
1:A:35:ILE:HG12	1:A:39:LYS:HE3	1.87	0.56
1:A:196:TYR:CE1	1:A:235:LEU:HB2	2.41	0.56
1:A:74:VAL:HG12	1:A:75:LYS:N	2.21	0.56
1:A:254:LEU:HD21	1:A:279:GLU:O	2.06	0.56
1:A:198:ASN:HB2	1:A:263:ARG:NH1	2.21	0.55
1:A:99:LEU:O	1:A:103:LEU:HG	2.05	0.55
1:A:220:GLY:HA3	1:A:235:LEU:CD2	2.37	0.55
1:A:236:LEU:HD21	1:A:276:ARG:NH2	2.21	0.54
1:A:23:THR:HB	1:A:57:VAL:HG21	1.90	0.54
1:A:91:ARG:HH22	1:A:140:GLU:HB3	1.71	0.54
1:A:81:TYR:HD2	1:A:111:VAL:HG12	1.72	0.53
1:A:241:LEU:HD22	1:A:252:PRO:HB2	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:LEU:O	1:A:102:THR:HB	2.07	0.53
1:A:132:ASP:C	1:A:134:HIS:H	2.17	0.52
1:A:259:TYR:CZ	1:A:263:ARG:HD2	2.44	0.52
1:A:66:ARG:HA	1:A:69:ILE:HD12	1.91	0.52
1:A:24:THR:HG23	1:A:55:TYR:CB	2.39	0.52
1:A:206:CYS:HB3	1:A:211:ILE:O	2.09	0.51
1:A:187:VAL:HG23	1:A:188:CYS:H	1.75	0.51
1:A:110:TYR:HB3	1:A:159:LEU:O	2.10	0.51
1:A:10:LEU:HD12	1:A:212:ILE:HD11	1.92	0.51
1:A:187:VAL:HG23	1:A:188:CYS:N	2.25	0.51
1:A:111:VAL:O	1:A:160:ALA:HA	2.11	0.51
1:A:46:PHE:HE2	1:A:277:ILE:HG22	1.77	0.50
1:A:46:PHE:CE2	1:A:277:ILE:HG22	2.46	0.50
1:A:74:VAL:HG12	1:A:75:LYS:H	1.77	0.50
1:A:258:ARG:HD3	1:A:283:VAL:O	2.12	0.50
1:A:55:TYR:O	1:A:57:VAL:HG23	2.11	0.49
1:A:165:VAL:HG23	1:A:189:ASN:OD1	2.12	0.49
1:A:99:LEU:HD21	1:A:160:ALA:HB2	1.94	0.49
1:A:112:ASP:HA	1:A:161:LYS:HB3	1.95	0.49
1:A:91:ARG:CZ	1:A:140:GLU:HB3	2.43	0.49
1:A:173:LEU:HD23	1:A:205:TYR:HE2	1.78	0.49
1:A:251:THR:CG2	1:A:252:PRO:HD2	2.44	0.48
1:A:91:ARG:O	1:A:94:LEU:HG	2.13	0.48
1:A:145:CYS:HB3	1:A:179:LYS:HD2	1.96	0.48
1:A:66:ARG:HG2	1:A:108:LEU:HD12	1.96	0.48
1:A:144:ILE:HG12	1:A:176:ILE:HD11	1.95	0.47
1:A:54:LEU:HD12	1:A:128:PHE:HD2	1.79	0.47
1:A:122:LEU:HA	1:A:139:PHE:HA	1.96	0.47
1:A:209:LYS:O	1:A:211:ILE:HG13	2.13	0.47
1:A:66:ARG:NH1	1:A:69:ILE:HD13	2.29	0.47
1:A:51:SER:O	1:A:84:LYS:HD2	2.15	0.47
1:A:24:THR:HG23	1:A:55:TYR:HB2	1.96	0.47
1:A:47:ARG:HH11	1:A:47:ARG:HG3	1.78	0.47
1:A:42:ILE:HA	1:A:46:PHE:O	2.15	0.46
1:A:143:ASP:HB3	1:A:146:ASP:HB2	1.98	0.46
1:A:213:LEU:O	1:A:265:VAL:HG13	2.15	0.46
1:A:54:LEU:HD22	1:A:86:TRP:CH2	2.50	0.46
1:A:251:THR:HG23	1:A:252:PRO:HD2	1.96	0.46
1:A:145:CYS:SG	1:A:175:ARG:HD2	2.56	0.46
1:A:102:THR:HG21	1:A:114:TYR:HE1	1.80	0.46
1:A:296:LEU:C	1:A:298:GLY:H	2.24	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:GLN:HE21	1:A:107:GLN:HA	1.81	0.45
1:A:38:THR:O	1:A:42:ILE:HD12	2.17	0.45
1:A:24:THR:HG23	1:A:55:TYR:CG	2.52	0.45
1:A:52:ALA:HB2	1:A:84:LYS:HD3	1.99	0.45
1:A:74:VAL:HG11	1:A:79:ILE:HD13	1.99	0.45
1:A:258:ARG:HH21	1:A:287:GLN:C	2.24	0.45
1:A:68:LYS:HE2	1:A:71:ASP:OD1	2.17	0.45
1:A:89:PHE:HA	1:A:94:LEU:HD11	1.99	0.45
1:A:86:TRP:HA	1:A:86:TRP:CE3	2.53	0.44
1:A:12:ASP:HB2	1:A:14:ASN:HD22	1.83	0.44
1:A:116:ILE:O	1:A:166:SER:HB2	2.17	0.44
1:A:145:CYS:SG	1:A:175:ARG:CD	3.06	0.44
1:A:258:ARG:NH2	1:A:288:LEU:HB2	2.32	0.44
1:A:156:ASP:HB2	1:A:184:TYR:CE2	2.52	0.44
1:A:76:ARG:NH2	1:A:79:ILE:HG22	2.33	0.44
1:A:81:TYR:H	1:A:112:ASP:HB2	1.83	0.43
1:A:279:GLU:O	1:A:282:GLN:HB2	2.19	0.43
1:A:128:PHE:CD1	1:A:128:PHE:N	2.86	0.43
1:A:10:LEU:HD12	1:A:212:ILE:CD1	2.49	0.43
1:A:213:LEU:HD23	1:A:214:VAL:O	2.18	0.43
1:A:280:LEU:O	1:A:283:VAL:HG13	2.17	0.43
1:A:10:LEU:HD13	1:A:16:ILE:HB	2.01	0.43
1:A:249:LYS:CE	1:A:250:GLN:HG2	2.46	0.43
1:A:166:SER:O	1:A:168:PHE:HD1	2.02	0.42
1:A:106:THR:HB	1:A:108:LEU:HB2	2.01	0.42
1:A:40:ILE:HD12	1:A:274:ALA:HA	2.01	0.42
1:A:194:HIS:HB3	1:A:218:THR:HA	2.02	0.42
1:A:34:VAL:HG11	1:A:57:VAL:CG1	2.49	0.42
1:A:90:HIS:O	1:A:142:VAL:HG21	2.20	0.42
1:A:199:GLN:HB2	1:A:202:MET:HB2	2.02	0.42
1:A:3:SER:O	1:A:4:ILE:HG13	2.20	0.41
1:A:111:VAL:HG21	1:A:114:TYR:HD1	1.85	0.41
1:A:10:LEU:CD1	1:A:16:ILE:HB	2.51	0.41
1:A:288:LEU:CD2	1:A:293:MET:HG2	2.51	0.41
1:A:119:PRO:HG2	1:A:172:GLN:NE2	2.23	0.41
1:A:128:PHE:N	1:A:128:PHE:HD1	2.19	0.41
1:A:144:ILE:HD11	1:A:168:PHE:CE2	2.55	0.41
1:A:187:VAL:O	1:A:211:ILE:HA	2.21	0.40
1:A:148:TRP:O	1:A:152:GLU:HG3	2.21	0.40
1:A:259:TYR:CE1	1:A:293:MET:SD	3.14	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	306/308 (99%)	227 (74%)	53 (17%)	26 (8%)	0 3

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	ILE
1	A	11	ASN
1	A	26	PRO
1	A	58	GLU
1	A	76	ARG
1	A	170	CYS
1	A	232	SER
1	A	250	GLN
1	A	302	ASN
1	A	161	LYS
1	A	197	LEU
1	A	210	ASP
1	A	225	LYS
1	A	272	PHE
1	A	283	VAL
1	A	205	TYR
1	A	300	ASN
1	A	70	GLU
1	A	251	THR
1	A	66	ARG
1	A	95	VAL
1	A	239	PRO
1	A	222	SER
1	A	271	SER
1	A	298	GLY
1	A	40	ILE

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	274/276 (99%)	198 (72%)	76 (28%)	0 2

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ASP
1	A	6	LEU
1	A	7	ARG
1	A	8	VAL
1	A	19	LEU
1	A	26	PRO
1	A	27	GLU
1	A	31	LYS
1	A	36	LYS
1	A	38	THR
1	A	40	ILE
1	A	42	ILE
1	A	44	ASN
1	A	48	HIS
1	A	56	GLU
1	A	58	GLU
1	A	61	VAL
1	A	68	LYS
1	A	69	ILE
1	A	70	GLU
1	A	73	THR
1	A	75	LYS
1	A	76	ARG
1	A	77	GLU
1	A	79	ILE
1	A	85	LEU
1	A	90	HIS
1	A	93	GLU
1	A	99	LEU
1	A	101	LYS

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Mol	Chain	Res	Type
1	A	102	THR
1	A	106	THR
1	A	107	GLN
1	A	108	LEU
1	A	111	VAL
1	A	122	LEU
1	A	127	ILE
1	A	131	ARG
1	A	137	LEU
1	A	142	VAL
1	A	153	LYS
1	A	155	LYS
1	A	163	ILE
1	A	169	ASN
1	A	170	CYS
1	A	178	ASN
1	A	179	LYS
1	A	180	PRO
1	A	182	LEU
1	A	190	GLN
1	A	191	VAL
1	A	201	LYS
1	A	203	LEU
1	A	213	LEU
1	A	226	THR
1	A	229	ASP
1	A	233	PRO
1	A	235	LEU
1	A	236	LEU
1	A	237	ASP
1	A	238	ASP
1	A	242	CYS
1	A	244	ILE
1	A	246	LYS
1	A	249	LYS
1	A	257	LEU
1	A	277	ILE
1	A	280	LEU
1	A	282	GLN
1	A	287	GLN
1	A	290	SER
1	A	291	GLU

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Mol	Chain	Res	Type
1	A	293	MET
1	A	301	ARG
1	A	306	ASN
1	A	307	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
1	A	14	ASN
1	A	44	ASN
1	A	63	GLN
1	A	107	GLN
1	A	172	GLN
1	A	190	GLN
1	A	306	ASN
1	A	307	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.